Supporting Information

Rationally Designed Synthesis of Bright Cu-Ga-Zn-Se-based Nanocrystals for Efficient Green Light-Emitting Diodes

Ruixin Sun,^{‡a} Jinxing Zhao,^{‡a} Ouyang Lin,^a Yu Li,^a Xiulin Xie,^a Wentao Niu,^a Zhe Yin,^{a*} and Aiwei Tang^{a*}

a Key Laboratory of Luminescence and Optical Information, Ministry of Education, School of Physical Science and Engineering, Beijing Jiaotong University, Beijing 100044, China

‡ These authors contributed equally to this work.

E-mail: awtang@bjtu.edu.cn; yinzhe@bjtu.edu.cn



Fig. S1 TEM images of CGZSe/ZnS NCs prepared under various Cu:Ga ratios. (a) 1:3, (b) 1:5, (c) 1:10, (d) 1:12, (e) 1:15.



Fig. S2 Evolution of the (a) absorption and PL spectra, (b) Comparison of PLQY and FWHM, (c) size distributions, (d) and ICP-MS characterization of CGZSe/ZnS NCs.



Fig. S3 XPS results of CGZSe/ZnS NCs (a) Cu 2p, (b) Ga 2p, (c) Se, (d) Zn 2p, (e) S 2p and Se 3p.



Fig. S4 TEM images of CGZSe NCs with different Zn. (a) 0 mmol, (b) 0.2 mmol, (c) 0.5 mmol, (d) 1.0 mmol and corresponding CGZSe/ZnS NCs, (e) 0 mmol, (f) 0.2 mmol, (g) 0.5 mmol, (h) 1.0 mmol.



Fig. S5 (a) Current density - luminance - voltage characteristic curves, (b) External quantum efficiency and current efficiency vary with luminance curves of QLEDs



constructed from CGZSe/ZnS NCs with different Zn.

Fig. S6 (a) Absorption and PL spectra (λ_{ex} =325 nm), (b) XRD patterns and TEM images

of CGZSe/ZnS with different kinds of Zn source. (c) ZnI_2 , (d) $Zn(St)_2$, (e) $Zn(OAc)_2$.



Fig. S7 (a) Band gaps of CGZSe/ZnS NCs. UPS spectra of the (b) high-binding energy electron cutoff, (c) valence-band edge regions with different Zn injection amounts.



Fig. S8 CGZSe/ZnS NCs with different Zn component as EML for QLEDs. (a)(d) EL spectra, (b)(e) current efficiency and EQE, (c)(f) J-L-V characteristic.

Sample	Element	1-0.5h	1-1h	2-0.5h	2-1h
CGZSe/ZnS NCs	Cu	2.0%	1.65%	1.5%	1.4%
	Ga	12.2%	10.5%	9.2%	9.7%
	Zn	85.8%	87.9%	89.3%	88.9%

Table S1. Element atomic ratio (ICP analysis) of CGZSe/ZnS NCs

Table S2. PL decay components for CGZSe/ZnS NCs

Sample	$ au_1/\mathrm{ns}$	α_1	$ au_2/\mathrm{ns}$	α_2	τ₃/ns	a3	$ au_{avg}/\mathrm{ns}$
Zn:0	129.8	22.5%	43.3	20.6%	940.1	56.9%	325.2
Zn:0.2	21.3	2.6%	131.1	52.1%	436.6	45.3%	246.2
Zn:0.5	17.8	1.6%	154.6	46.6%	476.4	51.8%	318.5
Zn:1	29.2	0.7%	202.6	43.7%	580.0	55.6%	398.4

Table S3. Performance of the green-emitting CGZSe/ZnS NCs-based QLEDs

Sample	EL peak	EQE _{max}	L _{max}	CE(ad/A)
	(nm)	(%)	(cd/m ²)	CE (CU/A)
ZnS:8+4	533	2.3	1103	7.2
ZnS:6+3	534	5.8	7016	18.4
ZnS:5+2.5	534	0.6	2615	1.9
ZnS:4+2	534	0.7	2287	2.2

Sample	EL peak	EQE _{max}	L _{max}	
	(nm)	(%)	(cd/m ²)	CE (CU/A)
ZnS:8+4	533	2.3	1103	7.2
ZnS:8	539	1.9	1540	5.5
ZnS:6+3	534	5.8	7016	18.4
ZnS:6	534	1.2	4810	3.7

Table S4. Performance of the green-emitting CGZSe/ZnS NCs-based QLEDs